

## **In situ FTIR investigations at varying temperatures on hydrous components in rutile**

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### **ABSTRACT**

In situ high- and low-temperature unpolarized FTIR absorption spectra of hydrous components in natural Fe-rich rutile have been recorded using a FTIR600 heating and cooling stage attached to an IR microscope. Two absorption bands ( $3279$  and  $3297\text{ cm}^{-1}$ ) at room temperature are ascribed to fundamental stretching bands of OH. Both OH bands shift to lower wavenumbers at elevated temperatures, but with different amplitudes. With increasing temperature, the integral absorbance of the  $3279\text{ cm}^{-1}$  band increases while the integral absorbance of the  $3297\text{ cm}^{-1}$  band decreases. These changes are fully reversible. The different frequency shifts of the two IR absorption bands with temperature imply two different local chemical environments of H defects. Based on the chemical composition of the rutile and the electronegativity of impurity ions, the results of the in situ high- and low-temperature FTIR measurements support the band assignment of Bromiley and Hilairt (2005): the  $3279$  and  $3297\text{ cm}^{-1}$  bands are due to interstitial H decoupled from any substitutional defects, and H coupled to  $\text{Fe}^{3+}$  on the neighboring octahedral (Ti) site ( $\text{Fe}_{\text{Ti}}^{3+} + \text{H}_i^+ \leftrightarrow \text{Ti}_{\text{Ti}}^{4+}$ ), respectively. Variations in integral absorbance of the two bands suggest the transformation between decoupled H defects and coupled H defects as a function of temperature, possible due to some statistical relationship between the proportions of coupled and decoupled interstitial H dependent on the amount of heat energy applied to the system.

**Keywords:** OH, IR, varying temperatures, rutile